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6. AUTHOR(S)
Professors A. Madhukar, I. G. Rosen, R. K. Kalia, P. Vashishta, and C. Wang

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
University of Southern California
Dept. of Materials Science & Engineering
3651 Watt Way, VHE 506
Los Angeles, CA 90089-0241

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
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14. ABSTRACT
This document summarizes the salient features of the accomplishments made during the period July 1, 1999 - June 30, 2001, of the above-titled MURI grant. The accomplishments include: (i) design and successful experimental implementation of single input (microwave power) adaptive real-time control of CF_4/O_2 plasma etching of Si_xN_y utilizing spectroscopic ellipsometry sensor feedback; (ii) development of highly efficient, dynamic load balancing, low overhead, and scalable algorithm to carry out atomistic simulations on massively parallel computing platforms and its testing for systems up to a billion atoms; (iii) multi-resolution molecular-dynamics simulations of atomic scale stress distributions and dislocation propagation in Si/Si_3N_4 nanopixels with up to 27 million atoms; (iv) developed a reflection-high-energy electron diffraction in-situ sensor based machine condition transfer function for reproducibility of molecular beam epitaxy (MBE) growth conditions; (v) examination of MBE growth on patterned surfaces and the role of surface stress engineering to achieve spatially selective growth of quantum dots; (vi) large scale molecular dynamics simulations of bare and overlayer covered nanoscale square mesas of the Ge/Si (001) and InAs/GaAs (001) systems; (vii) evidence from the InAs on GaAs (001) simulated stress relaxation for the observed self-limiting InAs overlayer thickness on GaAs nanomesas.

15. SUBJECT TERMS
Semiconductor manufacturing, in-situ sensors, real-time etching control, spectroscopic ellipsometry, molecular beam epitaxy, focused ion beam, nanostructures, silicon nitride, gallium arsenide, molecular dynamics, stresses in device nanomesas.

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Final Technical Report

July 1, 1995 – June 30, 2001

MURI '94 Program on
Process Modeling & In-Situ Sensor Feedback Based Adaptive Control of Molecular Beam Epitaxy and Ion-Assisted Reactive Etching of Advanced Semiconductor Structures

Contract No. F49620-95-1-0452

Submitted to

Dr. Marc Jacobs
Dr. Belinda King
Air Force Office of Scientific Research

Submitted by

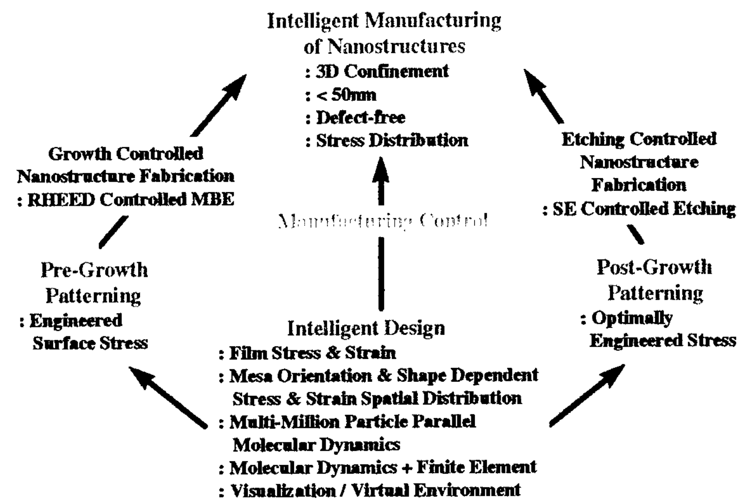
Anupam Madhukar
Principal Investigator
University of Southern California
Los Angeles, CA 90889-0241

Co-PIs
P. Chen
R. K. Kalia
I. G. Rosen
P. Vashishta
C. Wang

This document summarizes the objectives and salient accomplishments of the work undertaken under the above-noted MURI program.

I. Recalling Objectives

The joint efforts of researchers at the University of Southern California and Louisiana State University were focused upon understanding the scientific underpinnings and advancing the technological development of the paradigms and methodologies for in-situ sensor based control of growth and etching processes underlying semiconductor nanostructure fabrication, accounting for the synergism between nanostructure size/shape/orientation and the surface/interface mechanical stress inhomogeneities. The flow chart below depicts the two approaches to nanostructures synthesis: (a) pixellation via post-growth patterning and etching; (b) purely growth-controlled nanostructure synthesis via growth on pre-patterned substrates.



The focused objectives pertaining to these two complementary approaches were:

1. Real-time adaptive control of semiconductor/dielectric etching using Spectroscopic Ellipsometry (SE) / Optical Emission (OE) *in-situ* sensor feed-back
2. Growth-controlled nanostructure synthesis via control of molecular beam epitaxical growth on patterned and planar substrates using RHEED (reflection high-energy electron diffraction) in-situ sensor for run-to-run and machine-to-machine reproducibility of growth conditions.
3. Multimillion atom, massively parallel molecular dynamics based simulations of the spatially inhomogeneous stresses and strains in nanoscale ($\leq$ 50nm) mesas as a function of mesa orientation, shape and size.

These overall objectives involved achieving several sub-objectives that include physical modeling and simulation of selected processes and process consequences, developing empirical or phenomenological control models based upon *in-situ* sensor response, developing the algorithms and hardware to implement and test such control, developing multi-resolution (in space and time) scalable O(N) algorithms for molecular dynamics on massively parallel computing platforms, developing efficient algorithms for visualization of the massive data

generated, and developing and validating inter-atomic potential energy functions that represent the interactions in molecular dynamics simulations of semiconductor nanostructures.

II. Salient Accomplishments:

We summarize below the major accomplishments of this MURI project. These are divided into four categories relating to experiment and simulation, respectively, for each of the two approaches to nanostructure fabrication: post-growth pixellation and growth on pre-patterned mesas.

II.1 In-Situ Sensor based Real-time Adaptive Feedback Control of Semiconductor Etching

1. Developed a database and a phenomenological model of the thermal chlorine etch rate for GaAs as a function of substrate temperature and Cl_2 pressure (see publication 24).

2. Designed, simulated, tested, and successfully implemented a real time, adaptive feedback controller for thermal chlorine etching of gallium arsenide with spectroscopic ellipsometry sensing, accounting for a physically based model for the chamber valve (i.e. actuator) dynamics. The phenomenological model for the etch rate as a function of substrate temperature and Cl_2 pressure, noted under point 1 above, is utilized for adaptive control (see publications 21, 24, 37, 57, and 58).

3. Developed an artificial neural network (ANN) based approach to determining, from a limited data set, a process recipe that minimizes the sensitivity of the process output to errors in the machine sensors and actuators and implemented this methodology for the plasma enhanced chemical vapor deposition of silicon nitride dielectric films (see publications 32 and 52).

4. Carried out a 4 input variable full-factorial design-of-experiment (DoE) screening study of $CF_4/5\%O_2$ plasma etching of silicon nitride. The results indicated that microwave power and chamber pressure are the two most critical machine inputs for this plasma etch process.

5. Refined design, simulated, tested, and successfully implemented in-situ spectroscopic ellipsometry sensor based real-time, single input adaptive feedback controller for CF_4/O_2 plasma etching of silicon nitride. *Achieved a 60% improvement in machine reproducibility for the silicon nitride etch process* (see publications 30, 44, 45, and 57).

6. Designed and simulation tested two input (microwave power and chamber pressure) adaptive controller for CF_4/O_2 plasma etching of silicon nitride.

II.2. Si/Si_xN_y Nanopixel Stress Simulations:

1. Developed and validated the first interatomic potentials for Si/SixNy interface.

2. Developed highly efficient, dynamic load balancing, low overhead, and scalable algorithm to map irregular atomistic simulations on massively parallel machines and tested it for systems containing up to 1.04 billion atoms.

3. The first multiresolution molecular-dynamics simulations containing 4, 10 and 27 million atoms were performed on parallel computers to determine atomic -level stress distributions in 25nm, 54nm and 70nm nanopixel respectively, on a 0.15 μm silicon substrate. Effects of surfaces, edges, and lattice mismatch at the silicon/silicon nitride interface on the stress distribution were investigated. Compared to the crystalline silicon nitride case, the stress in

amorphous silicon nitride is highly inhomogeneous in the plane of the interface - a triangular lattice of stress domains of size 10 nm is observed (see publications 23, 36, 38, 42, and 46).

4. Mechanical behavior of the silicon/silicon nitride interface was also studied using million atom molecular dynamics simulations. At the critical value of the strain parallel to the interface, a crack forms on the silicon nitride surface and moves toward the interface. Time evolution of dislocation emission and nature of defects was studied in atomic detail and the speed of dislocation motion was determined to be 500 m/s (see publication 47).

II.3. Growth Controlled Semiconductor Nanostructures:

1. Developed and tested the methodology and algorithm (software) for determining MBE machine condition transfer function (MCTF) based upon GaAs substrate static surface RHEED specular beam intensity data as a function of the substrate temperature and arsenic pressure. This includes both discrete RHEED intensity representation via an adaptive grid based cubic spline fitting (i.e. system identification) and the mapping of the current and reference response surfaces into each other (i.e. system optimization) (see publications 19 and 31).

2. Use of Ga^+ implanted Si_xN_y as a negative resist for UHV patterning of Si_xN_y and pattern transfer to underlying GaAs upon which MBE growth controlled nanostructures are created (see publication 7).

II.4. Nanoscale Buried Structures and Overlayer-on-Mesa Stress Simulations:

1. Utilizing molecular dynamics simulations of the Ge/Si system as a vehicle, found that the growth – controlled pyramidal three-dimensional island nanostructures formed during strained epitaxy, when buried by an appropriate overlayer, give rise to a stress at the overlayer surface that varies inversely with the distance from the island center and scales essentially with the surface area of the island. This is in stark contrast to the inverse cubic distance dependence, and scaling with the buried object volume, found for spherical objects, the model that is most commonly employed to examine the nature and consequences of buried nanostructure (i.e. quantum dot) stress and strain (see publication 55).

2. Developed and validated inter-atomic potentials for GaAs, AlAs, InAs, and their pseudo-binary alloys to enable meaningful molecular dynamics simulations of nanostructures made of these technologically important semiconductors.

3. Performed multi-million atom molecular dynamics simulations to examine strain relaxation in InAs overlayers on GaAs(001) square mesas to shed light on the self-limiting growth we found experimentally. As a function of overlayer thickness, the in-plane lattice constant of InAs parallel to the InAs/GaAs(001) interface is found to begin to exceed that of the InAs bulk value at 12 monolayers (ML). The corresponding hydrostatic stress in the overlayer revealed a change from compressive to tensile. This is consistent with our experimentally observed self-limiting InAs overlayer thickness of~12ML for mesa linear dimensions ~100nm (see publications 54 and 56).

III. Personnel:

The list of senior researchers comprises the PI, Co-PIs, and senior postdocs as noted below:

A. Madhukar (PI)

P. Chen (Co-PI)

R. K. Kalia (Co-PI)

I. G. Rosen (Co-PI)

C. Wang (Co-PI)

R. Viswanathan

M. E. Bachlechner

Under this MURI, 10 Ph.D. and seven Master's degree students were fully or partially supported (the last graduate student who got started with MURI support is to graduate in Aug.2002). Additionally, 6 post doctoral fellows were supported. Of the Ph.D.'s graduated, 4 are now working in semiconductor manufacturing R&D at Intel, Motorola, Conexant; 4 in modeling/high performance computing, and 1 in finance industry. Of the MS graduates, 6 are working in industry and one continuing with PhD. Of the 6 Post Docs, 3 are in industry, 2 in faculty positions, and 1 in a government laboratory.

IV. List of Publications:

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V. Interactions / Transitions

(a). Participation/Presentations at Conferences, Seminars, etc.

Between the PI, Co-PIs, and postdocs, this MURI team made over 50 invited presentations at various national and international conferences and academic, industrial, and government laboratories. Additionally, over 20 contributed presentations at conferences were made.

(b) External Interactions / Knowledge Transfer

The most important transition of knowledge / research results has been in the form of the trained Ph.D. students and postdocs hired by the semiconductor industry (see numbers below). Specifically, Tyler Parent, who did his Ph.D. on spectroscopic ellipsometry based adaptive real time control of plasma etching, was hired by Intel where he continues to push the frontiers of etching; likewise, Amol Kalburge, who did his Ph.D. on in-situ focused ion beam assisted patterning and subsequent growth controlled nanostructure formation joined Conexant where he is in charge of developing the front end etching processes; as a third example, Timothy Campbell, who did his Ph.D. on the massively parallel molecular dynamics simulations is now working at NAVO, a DoD_MSRC high performance computing site in Mississippi.

Additionally, external interactions occurred with the following:

1. Motorola, with Ceramics Division in Phoenix, Arizona.

2. Argonne National Laboratory, concerning neutron scattering and MD studies of silicon nitride.

3. LSI Logic, Inc. concerning plasma process real time monitoring and control.

4. Intel Corp., concerning plasma process modeling, monitoring, and control.

5. Air Force Wright-Patterson Lab., concerning scalable parallel molecular dynamics and in-situ monitoring of MBE growth.

6. Air Force Philips Lab., concerning molecular dynamics simulations.

Amongst the postdocs trained, Ravi Viswanathan was lured away by then Rockwell (now Conexant) where he has been leading one of the semiconductor processing groups, and another postdoc, Rajesh Krishnamurthy, was hired away by Nortel, also for his expertise in semiconductor processing acquired as part of this MURI efforts.

VI. Honors/Recognition:

- DARPA Sustained Excellence Performer Award, USC-LSU MURI Team, Ultra Electronics Program, 1997.